

Theoretical Evidence for Equivalence between the Ground States of the Strong-Coupling BCS Hamiltonian and the Antiferromagnetic Heisenberg Model

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(Dated: February 2, 2008)

By explicitly computing wavefunction overlap via exact diagonalization in finite systems, we provide evidence indicating that, in the limit of strong coupling, i.e., $\Delta/t \rightarrow \infty$, the ground state of the Gutzwiller-projected BCS Hamiltonian (accompanied by proper particle-number projection) is identical to the exact ground state of the 2D antiferromagnetic Heisenberg model on the square lattice. This identity is adiabatically connected to a very high overlap between the ground states of the projected BCS Hamiltonian and the t - J model at moderate doping.

PACS numbers:

One of the key questions regarding high T_C superconductivity is whether it is possible for a repulsive electron-electron interaction alone to give rise to superconductivity. Considering that (i) the Hubbard model can be transformed into the t - J model in the limit of large on-site repulsion, and (ii), at half filling, the t - J model reduces to the two-dimensional (2D) $S = 1/2$ antiferromagnetic Heisenberg model with nearest-neighbor exchange coupling on the square lattice, the answer to the above question seems to lie in the relationship between 2D quantum antiferromagnetism and superconductivity. Although there is a consensus that the ground state of the 2D antiferromagnetic Heisenberg model has Néel order, i.e., staggered spin order [1], the precise nature of the ground state wavefunction itself, especially upon doping, is controversial.

The resolution of controversy requires both an *unbiased* and *unambiguous* study. Many analytic approaches are based on uncontrolled approximations such as the large- N expansion [2]. Even numerical approaches such as variational Monte Carlo simulation [3, 4] are biased by the choice of trial state which is assumed to be the ground state. Exact diagonalization, on the other hand, is a completely unbiased approach. However, its application is limited to finite systems with relatively small spatial size. This limitation generates a problem since the evidence of an ordered state is usually given by correlation functions. In the case of superconductivity, the relevant correlation function is the pairing correlation function: $F_{\alpha\beta}(\mathbf{r} - \mathbf{r}') = \langle c_{\uparrow}^{\dagger}(\mathbf{r})c_{\downarrow}^{\dagger}(\mathbf{r} + \alpha)c_{\downarrow}(\mathbf{r}')c_{\uparrow}(\mathbf{r}' + \beta) \rangle$ where $\alpha, \beta = \hat{x}, \hat{y}$. Off-diagonal long-range order can be claimed only when $F_{\alpha\beta}$ remains non-zero in the limit of large $|\mathbf{r} - \mathbf{r}'|$. Unfortunately, small spatial sizes of finite systems accessible via exact diagonalization make the distinction between true long-range order and short-range order (present even in normal states) ambiguous.

Despite the small spatial size, however, the size of Hilbert space is quite large; depending on the number of holes, there are 10^3 - 10^5 basis states in the 4×4 lattice system (even after translational symmetries are imple-

mented as reported in this paper). Since the ground state is constructed out of a very large number of possible linear combinations of basis states, it is a highly non-trivial task to infer a good ansatz wavefunction for the ground state itself. Consequently, if there is a method to show directly that some form of the BCS wavefunction is identical to the exact ground state of the 2D antiferromagnetic Heisenberg model, it will provide convincing evidence for superconductivity upon doping. In this paper, we put forward such a method: we compute the wavefunction overlap between the ground states of the t - J model and the Gutzwiller-projected BCS Hamiltonian via exact diagonalization. It should be emphasized that, in this paper, the Gutzwiller projection is applied directly in the BCS Hamiltonian instead of being applied onto the BCS ground state wavefunction. Note that the Gutzwiller-projected BCS wavefunction was originally proposed by Anderson [5] as a candidate for the ground state either on the square lattice with sufficiently strong next-nearest-neighbor exchange coupling, or on the triangular lattice. The Gutzwiller-projected BCS wavefunction was then conjectured to be a good ground state for the t - J model on the square lattice at moderate, non-zero doping. The difference between the ground state of the Gutzwiller-projected BCS Hamiltonian and the Gutzwiller-projected BCS ground state is most crucial at half-filling, which will be discussed in detail later in this paper.

The inspiration for using wavefunction overlap comes from the fractional quantum Hall effect (FQHE). It is well accepted by now that all essential aspects of FQHE are explained by the composite fermion (CF) theory [6]. One of the main reasons why we can put unequivocal trust in the CF theory may be the amazing agreement between the exact ground state and the CF wavefunction: the overlap is practically unity for various short-range interactions including the Coulomb interaction [7]. In this paper, we would like to achieve the same methodological clarity for the t - J model crucial in establishing the CF theory.

Before we discuss computational details, it is illumi-

nating to note that the analogy with FQHE goes much deeper than just methodology. To gain a physical insight into why the CF wavefunction is so accurate, let us consider the Laughlin wavefunction [8] which is a subset of CF wavefunctions at special lowest-Landau-level filling factor $\nu = 1/(2p + 1)$ with p an integer; especially at $\nu = 1/3$, it is given by $\Psi_{1/3} = \prod_{i < j} (z_i - z_j)^3$ where $z = x + iy$. Trugman and Kivelson [9], and Haldane [10] showed that $\Psi_{1/3}$ is actually the exact ground state of a short-range interaction given by $\nabla^2 \delta(\mathbf{r})$. For the Coulomb interaction (relevant for experiments), the Laughlin state remains extremely close to the exact ground state, as shown by practically unity overlap. The breakthrough for the CF theory was achieved when Jain realized that the Laughlin state is actually composed of two parts: the Jastrow factor, $\prod_{i < j} (z_i - z_j)^2$ (dubbed flux quanta attachment because of concomitant phase winding), and a non-interacting fermionic wavefunction of new quasiparticles, i.e., composite fermions. The key physical point is that, once the short-range correlation is captured by the Jastrow factor, residual correlations can be treated as relatively weak long-range correlations which are much easier to handle.

In fact, the separation between short-range and long-range correlations can serve as a general method in attacking strongly-correlated problems. The main question is what type of short-range correlation exists in the specific problem at hand, and more importantly what functional form of Jastrow factor describes this short-range correlation. Since we are interested in the quantum antiferromagnetism, it is natural to ask what has been known conclusively in the context of short-range correlation in quantum antiferromagnetic models.

To this end, let us consider the 1D $S = 1/2$ quantum Heisenberg model. This model is important because its solution is exactly known for two important cases of nearest-neighbor and $1/r^2$ exchange coupling. For the nearest-neighbor exchange coupling, the Bethe ansatz solution [11] gives the exact ground state which, for a given spin configuration, has an amplitude equal to the product of plane-wave states of spin flip excitation with appropriate phase shift. Since the Bethe ansatz solution is basically a product of plane-wave states, it is encouraging to guess that some form of Fermi sea state might be closely related to the exact Bethe ansatz solution, which turns out to be precisely the case. Various numerical works [12, 13] as well as exact analytic studies [14] showed that, in addition to closeness in energy, the spin-spin correlation function of the Gutzwiller-projected Fermi sea state has a power-law behavior very similar to the exact result. Note that the Gutzwiller projection simply imposes the no-double-occupancy constraint. Furthermore, Haldane [15] and Shastry [16] proved that the Gutzwiller-projected Fermi sea state is the exact ground state of the 1D $S = 1/2$ Heisenberg model with $1/r^2$ exchange coupling.

Now, combined with the fact that the Gutzwiller projection is basically an implementation of strong on-site repulsion, the above-mentioned similarity leads to a conjecture that the Gutzwiller projection plays the role of a Jastrow factor providing the short-range correlation embedded in quantum antiferromagnetism. To support this, we compute the overlap between the ground states of the Gutzwiller-projected BCS Hamiltonian and the antiferromagnetic Heisenberg model (in general, the t - J model at non-zero doping). In fact, we will show that the ground state of the projected BCS Hamiltonian is identical to the exact ground state of the Heisenberg model in the limit of strong coupling. Also, the overlap is very high ($\sim 90\%$) in a realistic parameter range relevant to cuprates, which is adiabatically connected to the unity overlap in the aforementioned limit.

We begin our quantitative analysis by writing the Hamiltonian of the t - J model:

$$\begin{aligned} H_{t-J} &= \hat{P}_G (H_t + H_J) \hat{P}_G, \\ H_t &= -t \sum_{\langle i,j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}), \\ H_J &= J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - n_i n_j / 4), \end{aligned} \quad (1)$$

where \hat{P}_G is the Gutzwiller projection operator imposing the no-double-occupancy constraint. We obtain the exact ground state of H_{t-J} using a modified Lanczos method. We have checked that our results for the t - J model completely agree with previous numerical studies [17] for all available cases.

Now, let us turn our attention to the Gutzwiller-projected BCS Hamiltonian. As mentioned in the beginning, our approach is rather different from previous approaches [3, 4, 18, 19] which applied the number projection as well as the Gutzwiller projection onto the explicit BCS wavefunction. We do not take these previous approaches for two reasons. First, there is a singularity due to the spin-density-wave instability inherent in the BCS Hamiltonian with on-site repulsion, which generates Néel order at half filling. So, it is important to study directly the Gutzwiller-projected BCS Hamiltonian instead of applying the Gutzwiller projection onto the BCS ground state. The Gutzwiller-projected BCS Hamiltonian is given as follows:

$$\begin{aligned} H_{\text{BCS}} &= H_t + H_\Delta, \\ H_\Delta &= \Delta \sum_i (c_{i\uparrow}^\dagger c_{i+\hat{x},\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{i+\hat{x},\uparrow}^\dagger + \text{h.c.}) \\ &\quad - \Delta \sum_i (c_{i\uparrow}^\dagger c_{i+\hat{y},\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{i+\hat{y},\uparrow}^\dagger + \text{h.c.}), \\ H_{\text{BCS}}^G &= \hat{P}_G H_{\text{BCS}} \hat{P}_G, \end{aligned} \quad (2)$$

where H_t is given in Eq.(1). Note the sign change in front of Δ in the y direction compared to that of x direction:

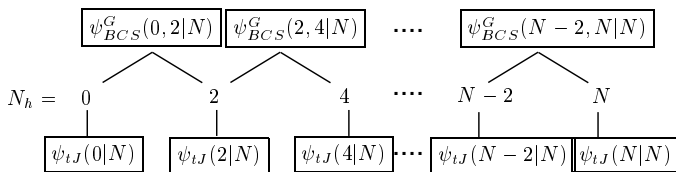


FIG. 1: Schematic diagram for constructing the ground state of the Gutzwiller-projected BCS Hamiltonian, $\psi_{BCS}^G(N_h, N_h + 2|N)$, and the exact ground state of the t - J model, $\psi_{t-J}(N_h|N)$. N_h (N) is the number of holes (sites).

the gap function is given in momentum space by $\tilde{\Delta}(\mathbf{k}) = 2\Delta(\cos k_x - \cos k_y)$. The Gutzwiller projection is built in from the onset by working solely in the Hilbert space with the no-double-occupancy constraint.

The second reason is rather subtle, but physically very important. Coherent number fluctuations (as opposed to incoherent fluctuations in the normal state) are ultimately responsible for the intrinsic properties of superconductivity. So, coherent number fluctuations should be incorporated even into finite-system studies in a fundamental manner. In essence, we diagonalize H_{BCS}^G in the combined Hilbert space of N_e and $N_e + 2$ particles. There is, however, a spurious finite-size effect which prevents pairing if one naively diagonalizes H_{BCS}^G in the combined Hilbert space. In finite systems, the energy cost of adding (removing) few particles is not negligible compared to the total energy. So, the mixing between states with even a few-particle difference is energetically prohibited. We fix this problem by adjusting the chemical potential so that the kinetic energy plus the chemical potential energy of the N_e particle ground state is the same as that of the $N_e + 2$ particle ground state, which eliminates a spurious energy penalty for pairing. Once the chemical potential is set, it can be shown that the mixing with other particle-number sectors such as the $N_e + 4$ sector is negligibly small, even if it is allowed.

Let us define the following notations: $\psi_{BCS}^G(N_h, N_h + 2|N)$ denotes the ground state of the Gutzwiller-projected BCS Hamiltonian obtained from the combined Hilbert space of N_h and $N_h + 2$ holes in the system of N sites. $\hat{\mathcal{P}}_{N_h=N_0}$ denotes the number projection operator which projects states onto the Hilbert space of N_0 holes and re-normalizes the projected states. $\psi_{t-J}(N_h|N)$ is the exact ground state of the t - J model in the Hilbert space of N_h holes in N sites. A schematic diagram is shown in Fig.1.

We now present our exact-diagonalization results of overlap for various numbers of holes in the 4×4 square lattice system with periodic boundary conditions. Note that the 4×4 system is one of the most studied systems in numerics [1] because it is accessible via exact diagonalization, yet large enough to contain essential many-body correlations. While it is possible to study all pos-

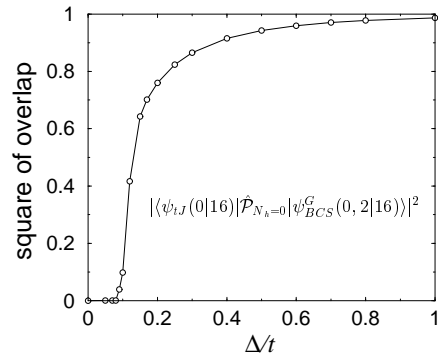


FIG. 2: Square of the overlap between the ground state of the projected BCS Hamiltonian, $\hat{\mathcal{P}}_{N_h=0}|\psi_{BCS}^G(0, 2|16)\rangle$, and the exact ground state of the t - J model, $|\psi_{t-J}(0|16)\rangle$, for the 0-hole case in the 4×4 system (undoped regime).

sible dopings in the 4×4 system, we concentrate on the three most important cases: 0 hole (undoped regime), 2 holes (optimally doped regime), and 4 holes (overdoped regime). Also, we study only an even number of holes since, in finite systems, an odd number of holes will artificially frustrate pairing order.

Let us begin with the 0-hole case, i.e., the 2D antiferromagnetic Heisenberg model. Though the numerical evidence for Néel order is quite convincing [1], our knowledge of the ground state itself is very limited, considering that (i) the semiclassical configuration of staggered spins is not the exact ground state, and (ii) there are still rather strong quantum fluctuations. So, it will be satisfactory if one can show that the ground state of the Gutzwiller-projected BCS Hamiltonian is a good representation of the exact ground state of the 2D antiferromagnetic Heisenberg model. The criterion for the effectiveness of the ground state of the projected BCS Hamiltonian is quantified via its overlap with the exact ground state of the Heisenberg model. High overlap will provide evidence for the existence of pairing which, in turn, generates superconductivity upon doping.

When Anderson [5] proposed the RVB state (which is a synonym for the projected BCS state), his insight was that electrons are already paired at zero doping, but the ground state cannot superconduct (for that matter, conduct) because there are no mobile charge carriers. It seems reasonable, then, that the ground state becomes superconducting as soon as holes are added. However, the idea of the RVB state as the ground state of the Heisenberg model was rejected because the RVB state does not have any long-range magnetic order, while the exact ground state has Néel order [20, 21]. The situation is quite different for the ground state of the Gutzwiller-projected BCS Hamiltonian. Fig.2 shows that, at zero doping, the ground state of the projected BCS Hamiltonian, $\hat{\mathcal{P}}_{N_h=0}|\psi_{BCS}^G(0, 2|16)\rangle$, is actually identical to the exact ground state of the t - J model, $|\psi_{t-J}(0|16)\rangle$, in the limit of $\Delta/t \rightarrow \infty$. Since the two states are identical,

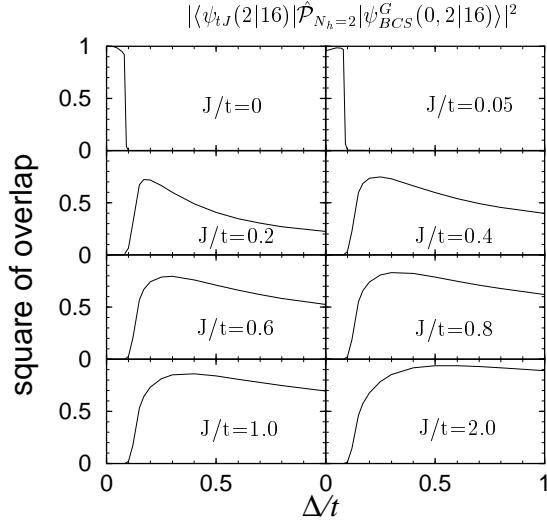


FIG. 3: Square of the overlap between the ground state of the projected BCS Hamiltonian, $\hat{\mathcal{P}}_{N_h=2}|\psi_{BCS}^G(0, 2|16)\rangle$, and the exact ground state of the t - J model, $|\psi_{t-J}(2|16)\rangle$, for the 2-hole case in the 4×4 system (optimally doped regime).

it is clear that the ground state of the projected BCS Hamiltonian has Néel order. This identity at infinite Δ/t is consistent with previous Monte Carlo simulations [4], in which their variational gap parameter becomes very large at small doping. It is important to know that the largeness of Δ/t does not necessarily mean strong superconductivity since, despite strong pairing, there is very little charge fluctuation at small doping [22].

But, physically, why is the overlap unity at infinite Δ/t , or equivalently $t = 0$? To answer this, consider the t - J Hamiltonian at zero doping, H_J , and the BCS Hamiltonian with $t = 0$, H_Δ . H_J contains $\mathbf{S}_i \cdot \mathbf{S}_j$ which prefers the formation of spin singlet pairs. Similarly, H_Δ contains $c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger$ which also prefers to create spin singlet pairs. So, provided that the no-double-occupancy constraint is imposed via Gutzwiller projection, H_J and H_Δ should have the same physical effect.

We now move onto the cases with finite doping. Since pairing already exists at zero doping, it is expected that the ground state becomes superconducting upon doping. We support this by showing that, in the Hilbert space of two holes, the ground state of the projected BCS Hamiltonian, $\hat{\mathcal{P}}_{N_h=2}|\psi_{BCS}^G(0, 2|16)\rangle$, has a very high overlap ($\sim 90\%$) with $|\psi_{t-J}(2|16)\rangle$ at optimal Δ/t for a realistic range of J/t : $0.4 \lesssim J/t \lesssim 0.8$ (middle panels in Fig.3 showing the square of the overlap). Note that Δ/t can be taken as a variational parameter. In fact, the optimal overlap approaches unity when J/t becomes sufficiently large (bottom, right in Fig.3). While the large J/t regime itself is not very realistic, the high overlap in the realistic regime is adiabatically connected to the unity overlap in the large J/t limit. Incidentally, the identity between ψ_{t-J} and ψ_{BCS}^G at $J/t = 0$ and $\Delta/t = 0$ (top, left in

Fig.3) is rather trivial because H_{t-J} and H_{BCS}^G become identical in this case. It is important to note that the nature of the identity at large J/t is completely different from that of zero J/t , as manifested by symmetry changes of the ground state. The t - J model ground state changes its rotational symmetry from s -wave to d -wave at $J/t \simeq 0.08$ while the ground state of the projected BCS Hamiltonian does so at $\Delta/t \simeq 0.1$. Therefore, the regime with large J/t and Δ/t is completely disconnected from the regime with small J/t and Δ/t . It is important to distinguish the rotational symmetry of the ground state from the pairing symmetry. The latter is always d -wave while the former changes as a function of Δ/t .

Finally, we have checked that, in the overdoped regime, the ground state of the projected BCS Hamiltonian is no longer a good representation of the ground state of the t - J model, which is supported by the negligible overlap between $\hat{\mathcal{P}}_{N_h=4}|\psi_{BCS}^G(2, 4|16)\rangle$ and $|\psi_{t-J}(4|16)\rangle$ for general parameter range.

In conclusion, we have provided evidence that, in the limit of strong coupling, the ground state of the Gutzwiller-projected BCS Hamiltonian is equivalent to that of the 2D antiferromagnetic Heisenberg model. Combined with high overlaps at moderate doping, this equivalence supports the existence of superconductivity in the t - J model. For future work, it will be interesting to investigate an analytic approach in proving the equivalence.

The author is very grateful to S. Das Sarma for his support throughout this work, and to J. K. Jain for his insightful comment on the difference between the projected Hamiltonian and the projected ground state. The author is also indebted to V. Galitski, D. J. Priour, Jr. and V. W. Scarola for valuable discussions. This work was supported by ARDA and NSF.

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- [1] For review, E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).
 - [2] E. Fradkin, *Field theories of condensed matter systems* (Addison-Wesley, 1991).
 - [3] C. Gros, Phys. Rev. B **38**, R931 (1988).
 - [4] A. Paramekanti *et al.*, Phys. Rev. Lett. **87**, 217002 (2001).
 - [5] P. W. Anderson, Science **235**, 1196 (1987).
 - [6] J. K. Jain, Phys. Rev. Lett. **63**, 199 (1989).
 - [7] For example, see the chapter by J. K. Jain in *Perspectives in Quantum Hall Effects*, edited by S. Das Sarma and A. Pinczuk (Wiley, New York, 1997).
 - [8] R. B. Laughlin, Phys. Rev. Lett. **50**, 1395 (1983).
 - [9] S. A. Trugman and S. Kivelson, Phys. Rev. B **31**, 5280 (1985).
 - [10] F. D. M. Haldane, Phys. Rev. Lett. **51**, 605 (1983).
 - [11] H. A. Bethe, Z. Physik **71**, 205 (1931).
 - [12] T. A. Kaplan *et al.*, Phys. Rev. Lett. **49**, 889 (1982).
 - [13] C. Gros *et al.*, Phys. Rev. B **36**, 381 (1987).
 - [14] F. Gebhard and D. Vollhardt, Phys. Rev. Lett. **59**, 1472

- (1987).
- [15] F. D. M. Haldane, Phys. Rev. Lett. **60**, 635 (1988).
 - [16] B. S. Shastry, Phys. Rev. Lett. **60**, 639 (1988).
 - [17] E. Dagotto *et al.*, Phys. Rev. B **45**, 10741 (1992).
 - [18] Y. Hasegawa and D. Poilblanc, Phys. Rev. B **40**, 9035 (1989).
 - [19] S. Sorella *et al.*, Phys. Rev. Lett. **88**, 117002 (2002).
 - [20] S. Chakravarty *et al.*, Phys. Rev. Lett. **60**, 1057 (1988).
 - [21] J. D. Reger and A. P. Young, Phys. Rev. B **37**, R5978 (1988).
 - [22] The true measure of superconductivity is $F_{\alpha\beta}$ in the limit of large $|\mathbf{r} - \mathbf{r}'|$, which can be shown quite generally to be proportional to the square of hole concentration at small doping for the projected BCS state [4].